

Locally optimal 2-periodic sphere packings

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Abstract

The sphere packing problem is an old puzzle. We consider packings with m spheres in the unit cell (m -periodic packings). For the case $m = 1$ (lattice packings), Voronoi presented an algorithm to enumerate all local optima in a finite computation, which has been implemented in up to $d = 8$ dimensions. We generalize Voronoi's algorithm to $m > 1$ and use this new algorithm to enumerate all locally optimal 2-periodic sphere packings in $d = 3, 4$, and 5 . In particular, we show that no 2-periodic packing surpasses the density of the optimal lattice in these dimensions. A partial enumeration is performed in $d = 6$.

Keywords: sphere packing, periodic point set, quadratic form, Ryshkov polyhedron

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1. Introduction

The sphere packing problem asks for the highest possible density achieved by an arrangement of nonoverlapping spheres in a Euclidean space of d dimensions. The exact solutions are known in $d = 2$ [1], $d = 3$ [2], $d = 8$ [3] and $d = 24$ [4].

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This natural geometric problem is useful as a model of material systems and their phase transitions, and, even in nonphysical dimensions, it is related to fundamental questions about crystallization and the glass transition [5]. The sphere packing problem also arises in the problem of designing an optimal error-correcting code for a continuous noisy communication channel [6]. Perhaps even more than the obvious applications of the sphere packing problem, contributing to its importance is the unexpected wealth of remarkable structures that appear as possible solutions and merit study in their own right [7, 8].

There does not appear to be a systematic solution or construction that achieves the optimal packing in every dimension, and every dimension seems to have its own quirks, unearthing new surprises [6]. In some dimensions, such as $d = 8$ and $d = 24$, the solution is unique and given by exceptionally symmetric lattices. In others, such as $d = 3$, there is a lattice that achieves the highest density, but this density can also be achieved by other periodic packings with larger fundamental unit cells and even by aperiodic packings. For $d = 10$ it seems that the highest density, achieved by a periodic arrangement with 40 spheres per unit cell, cannot be achieved by a lattice. In any given dimension, the densest packing known is periodic, but it is not known whether there is some dimension where the densest packing is not periodic. In fact, frighteningly little is known in general as we go up in dimensions. It is possible that in all dimensions the densest packing is achieved by a periodic packing with a universally bounded number of spheres in the unit cell, that in all dimensions it is achieved by a periodic packing, but only with unboundedly many spheres in the unit cell, or that in some dimension it is not achieved by a periodic packing at all. In any case, periodic packings with arbitrarily many spheres in the unit cell can approximate the optimal density in any dimension to arbitrary precision.

Therefore, it is reasonable to ask for the optimal density achieved by a periodic packing in d dimensions with m spheres per unit cell, which we denote $\phi_{d,m}$. In the limit $m \rightarrow \infty$, this density approaches (and possibly equals for some finite m) the optimal packing density ϕ_d . Apart from the dimensions where ϕ_d is known, there are no cases with $m > 1$ where $\phi_{d,m}$ is known. In this

paper, we describe a general method for calculating $\phi_{d,2}$, and use it to obtain $\phi_{4,2} = \phi_{4,1}$ and $\phi_{5,2} = \phi_{5,1}$. Our method could also be generalized to larger m , but becomes more complicated.

For the case $m = 1$, corresponding to lattices, Voronoi gave an algorithm to enumerate all the locally optimal solutions to the problem. In geometrical terms, Voronoi's algorithm uses the fact that the space of lattices up to isometry can be parameterized (redundantly) by positive definite quadratic forms. The subset in the linear space of quadratic forms that corresponds to lattices with no two points less than a certain distance apart is a polyhedron. The additional fact that the density of lattice points is a quasiconvex function implies that local maxima can only occur at the vertices of this polyhedron. Because there are only finitely many vertices that correspond to distinct lattices, the local optima of the lattice sphere packing problem can be fully enumerated. This interpretation of Voronoi's algorithm was suggested by Ryshkov [9] and so the polyhedron is known as the Ryshkov polyhedron. The lattices corresponding to vertices of the polyhedron are known as *perfect lattices*, but not every perfect lattice is locally optimal, or an *extreme lattice*. This algorithm has been implemented and executed to determine $\phi_{d,1}$ for $d \leq 8$, as well as to enumerate all perfect lattices in these dimensions [10]. However, the exploding number of perfect lattices as d increases make the execution of this algorithm currently unfeasible even for $d = 9$ [11].

Schürmann transported some of the concepts from Voronoi's theory to the case of periodic packings and was able to show that any extreme lattice, when viewed as a periodic packing, is still locally optimal [12, 13]. However the nonlinearities that arise in the case $m > 1$ have made it difficult to use this version of the theory to provide an analog of Voronoi's algorithm. In this paper we transport the concepts in a slightly different way than Schürmann, permitting us to reconstruct many of the elements of Voronoi's algorithm in the case of periodic packings with fixed m . These elements behave nicely enough for $m = 2$ to allow us to provide an algorithm for the enumeration of all locally optimal packings, and we execute this algorithm for $d \leq 5$.

2. Theoretical preparation

2.1. Periodic point sets

For a set of points, $\Xi \subset \mathbb{R}^d$, the *packing radius* is the largest radius, such that if balls were centered at each of the points, they would not overlap. Namely, the packing radius is half the infimum distance between any two points, $\rho(\Xi) = \frac{1}{2} \inf_{x, y \in \Xi} \|x - y\|$. A set of points is *periodic* if there are d linearly independent vectors $\mathbf{a}_1, \dots, \mathbf{a}_d$, such that the set is invariant under translation by any of these vectors. The group generated by $\mathbf{a}_1, \dots, \mathbf{a}_d$ is a lattice, $\Lambda = \{\sum_{i=1}^d n_i \mathbf{a}_i : n_1, \dots, n_d \in \mathbb{Z}\}$. If all translations that fix the set are in Λ , we say that Λ is a primitive lattice for the periodic set. The primitive lattice is unique. A set that is periodic under translation by a lattice Λ and has m orbits under translations by Λ called m -periodic. We will only deal with sets of positive packing radius, and therefore m is necessarily finite.

The number density of a periodic set Ξ is given by

$$\delta(\Xi) = \frac{m}{\det \Lambda}, \quad (1)$$

where $\det \Lambda$ is the volume of a parallelotope generated by the generators of Λ , $\{\sum_{i=1}^d x_i \mathbf{a}_i : 0 \leq x_1, \dots, x_d \leq 1\}$. This parallelotope and its translates under Λ tile \mathbb{R}^d , and its volume is the same as the volume of any other *fundamental cell* of Λ , that is, a polytope whose Λ -translates tile \mathbb{R}^d . Therefore, this is a property of Λ , and not of the particular basis. Also, since Λ itself is not uniquely determined from Ξ , but can be any sublattice of the primitive lattice of Ξ , it is important to note that the formula for $\delta(\Xi)$ above is independent of the choice of Λ . The largest density that can be achieved by a packing of equal-sized balls centered at the points of Ξ is $\phi(\Xi) = V_d \rho(\Xi)^d \delta(\Xi)$, where V_d is the volume of a unit ball in \mathbb{R}^d . In any family of point sets closed under homothety, such as periodic sets or m -periodic sets, maximizing the packing density ϕ is equivalent to maximizing the number density under the constraint $\rho(\Xi) \geq \rho_0$ for some fixed ρ_0 .

2.2. Voronoi's algorithm

A 1-periodic packing is a translate of a lattice. The packing radius of a lattice is given by

$$\rho(\Lambda) = \frac{1}{2} \min_{\mathbf{l}, \mathbf{l}' \in \Lambda} \|\mathbf{l} - \mathbf{l}'\| = \frac{1}{2} \min_{\mathbf{l} \in \Lambda} \|\mathbf{l}\|. \quad (2)$$

The packing radius of a lattice and the volume of its fundamental cell are both invariant under rotations of the lattice. Therefore, to find the densest lattice packing, we only need to consider lattices up to rotation. Consider a lattice $\Lambda = A\mathbb{Z}^d$ generated by $\mathbf{a}_1, \dots, \mathbf{a}_d$. The quadratic form $Q: \mathbb{Z}^d \rightarrow \mathbb{R}$, $Q(n_1, \dots, n_d) = \|n_1\mathbf{a}_1 + \dots + n_d\mathbf{a}_d\|^2$ determines Λ up to rotations. However, since a lattice can have different generating vectors, different quadratic forms can correspond to the same lattice. Q and Q' correspond to the same lattice if and only if $Q = Q \circ U$, where $U \in GL_d(\mathbb{Z})$. This is precisely the group of linear maps that map \mathbb{Z}^d to itself. The packing radius of a lattice Λ corresponding to the quadratic form Q is $\rho(\lambda) = \frac{1}{2}(\min Q)^{1/2}$, where $\min Q$ is the minimum of Q over nonzero vectors. The determinant of Λ is given by $(\det Q)^{1/2}$.

The linear space of quadratic forms can be identified with the linear space of symmetric matrices \mathcal{S}^d using the standard basis of \mathbb{Z}^d , so that $Q(\mathbf{n}) = \mathbf{n}^T Q \mathbf{n}$. And the natural inner product in this space is given by $\langle Q, Q' \rangle = \text{tr } QQ'$. The condition $\min Q \geq \lambda$ can be written as the intersection of infinitely many linear inequalities:

$$Q(\mathbf{n}) = \langle \mathbf{n}\mathbf{n}^T, Q \rangle \geq \lambda \quad \text{for all } \mathbf{n} \in \mathbb{Z}^d \quad (3)$$

It can be easily checked that for $\lambda > 0$, Eq. (3) implies that Q is a positive definite matrix, and a lattice corresponding to it can be recovered, e.g. by Cholesky decomposition. Ryshkov observed that the set $\{Q : \min Q \geq \lambda\}$, albeit an infinite intersection of linear inequalities, behaves locally like a finite intersection, namely a polyhedron, and therefore this set is known as the Ryshkov polyhedron [9]. Though the Ryshkov polyhedron has infinitely many vertices, there are only finitely many orbits under the action of $GL_d(\mathbb{Z})$. Therefore, by starting at some vertex, enumerating the vertices with which it shares an edge, and

repeating the process for any enumerated vertex not of the same orbit as a previous vertex, one can computationally enumerate all the orbits of vertices of the Ryshkov polyhedron. Since the determinant is a quasiconcave function, its local minima in the polyhedron can occur only on the vertices, and to find the global minimum it is enough to compare its value at all the vertices.

2.3. The Ryshkov-like Polyhedron

To parameterize m -periodic point sets, we can use a similar scheme. An m -periodic point set is the union of m translates of a lattice, $\Xi = \bigcup_{i=0}^{m-1} (\Lambda + \mathbf{b}_i)$, where $\Lambda = A\mathbb{Z}^d$. Without loss of generality, we can take $\mathbf{b}_0 = 0$. Now, consider the set $\mathcal{M} \subseteq \mathbb{Z}^{d+m-1}$ given by $\mathcal{M} = \mathbb{Z}^d \times (E - E)$, where $E = \{0, \mathbf{e}_1, \dots, \mathbf{e}_{m-1}\}$ is the standard basis of \mathbb{Z}^{m-1} plus the zero vector. We define the following function $J : \mathcal{M} \rightarrow \mathbb{R}$, which determines Ξ up to rotation:

$$J(n_1, \dots, n_d, l_1, \dots, l_{m-1}) = \|n_1 \mathbf{a}_1 + \dots + n_d \mathbf{a}_d + l_1 \mathbf{b}_1 + \dots + l_{m-1} \mathbf{b}_{m-1}\|^2. \quad (4)$$

This function can be extended uniquely to a quadratic form over \mathbb{R}^{d+m-1} , represented by a symmetric matrix $J \in \mathcal{S}^{d+m-1}$, namely

$$J = \begin{pmatrix} Q & R^T \\ R & S \end{pmatrix}, \quad (5)$$

where $Q_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j$, $R_{ij} = \mathbf{b}_i \cdot \mathbf{a}_j$, and $S_{ij} = \mathbf{b}_i \cdot \mathbf{b}_j$. The packing radius of Ξ is related to the minimum of the quadratic form. Namely, $\rho(\Xi) = \frac{1}{2}(\min J)^{1/2}$, where $\min J$ is the minimum of J over $\mathcal{M} \setminus \{0\}$. Let $\mathcal{R}(\lambda) = \{J : \min J \geq \lambda\}$. This set is defined as the intersection of linear inequalities:

$$J \in \mathcal{R}(\lambda) \quad \text{iff} \quad J(\mathbf{k}) = \langle \mathbf{k} \mathbf{k}^T, J \rangle \geq \lambda \quad \text{for all } \mathbf{k} \in \mathcal{M} \setminus \{0\}. \quad (6)$$

We want to show that $\mathcal{R}(\lambda)$, like the Ryshkov polyhedron, behaves locally like a polyhedron.

Lemma 1. *Let $Q : \mathbb{R}^d \rightarrow \mathbb{R}$ be a positive definite quadratic form, satisfying $Q(\mathbf{n}) \geq \lambda$ for all $\mathbf{n} \in \mathbb{Z}^d$ and $\text{tr} Q \leq C$. Then any vector $\mathbf{x} \in \mathbb{R}^d$ satisfying $Q(\mathbf{x}) \leq 1$ also satisfies $\|\mathbf{x}\| \leq M$, where M depends on d , λ , and C .*

The proof is given in Theorem 3.1 of [10].

Theorem 1. *Let $W = \{J \in \mathcal{R}(\lambda) : |J_{ij}| \leq L\}$. There are only finitely many $\mathbf{k} \in \mathcal{M}$ such that for some $J \in W$, $J(\mathbf{k}) \leq \lambda$.*

Proof. Let $\mathbf{k} = (\mathbf{n}, \mathbf{l})$. There are only finitely many choices for \mathbf{l} . So, we need only show that for any fixed choice of \mathbf{l} , there are finitely many $\mathbf{n} \in \mathbb{Z}^d$ such that $J(\mathbf{k}) \leq \lambda$ for some $J \in W$. We have

$$\begin{aligned} J(\mathbf{k}) &= \mathbf{n}^T Q \mathbf{n} + 2\mathbf{l}^T R \mathbf{n} + \mathbf{l}^T S \mathbf{l} \\ &= (\mathbf{n} + \mathbf{q})^T Q (\mathbf{n} + \mathbf{q}) + \mathbf{l}^T S \mathbf{l} - \mathbf{q}^T Q \mathbf{q}, \end{aligned} \tag{7}$$

where $\mathbf{q} = Q^{-1} R^T \mathbf{l}$. Therefore, if $J(\mathbf{k}) \leq \lambda$ then $(\mathbf{n} + \mathbf{q})^T Q (\mathbf{n} + \mathbf{q}) \leq \lambda + \mathbf{q}^T Q \mathbf{q} - \mathbf{l}^T S \mathbf{l} \leq \lambda + \mathbf{q}^T Q \mathbf{q} = \lambda + \mathbf{l}^T R Q^{-1} R^T \mathbf{l}$.

Since $\mathbf{l}^T R R^T \mathbf{l} \leq 4dL^2$ and $\text{tr} Q \leq dL$, we have from the lemma that $\mathbf{l}^T R Q^{-1} R^T \mathbf{l} \leq 4dL^2 M^2$. Therefore, if $J(\mathbf{k}) \leq \lambda$ then $(\mathbf{n} + \mathbf{q})^T Q (\mathbf{n} + \mathbf{q}) \leq \lambda + 4dL^2 M^2$. Again, from the lemma, we have that $(\mathbf{n} + \mathbf{q})^T (\mathbf{n} + \mathbf{q}) \leq \lambda M^2 + 4dL^2 M^4$. Therefore, there can only be finitely many choices of \mathbf{n} for each choice of \mathbf{l} such that $J(\mathbf{k}) \leq \lambda$ for some $J \in W$. \square

So, $\mathcal{R}(\lambda)$ is locally a polyhedron in the sense that any intersection of $\mathcal{R}(\lambda)$ with a bounded polyhedron is a bounded polyhedron. We call it the Ryshkov-like polyhedron.

2.4. Symmetries of the Ryshkov-like polyhedron

The symmetries of $\mathcal{R}(\lambda)$ are tightly linked with the symmetries of the set $\mathcal{M} \subset \mathbb{Z}^{d+m-1}$. Namely, if $T : \mathbb{R}^{d+m-1} \rightarrow \mathbb{R}^{d+m-1}$ is a linear map such that $T(\mathcal{M}) = \mathcal{M}$, then $J \mapsto J \circ T$ maps $\mathcal{R}(\lambda)$ to itself.

We decompose T into blocks with a top-left block of size $d \times d$. It is easy to see that the bottom-left block must be zero, or else there is always some $\mathbf{k} \in \mathcal{M}$ such that $T(\mathbf{k}) = (\mathbf{n}, \mathbf{l})$, where $\mathbf{l} \notin (E - E)$. Therefore we write

$$T = \begin{pmatrix} U & V \\ 0 & W \end{pmatrix}. \tag{8}$$

As a consequence, we also have that U and W must be invertible as maps $\mathbb{Z}^d \rightarrow \mathbb{Z}^d$ and $(E - E) \rightarrow (E - E)$. Therefore, $U \in GL_d(\mathbb{Z})$ and W is a permutation of E , namely

$$W = \begin{pmatrix} 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \Pi \begin{pmatrix} -1 & -1 & \cdots \\ 1 & 0 & \cdots \\ 0 & 1 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \quad (9)$$

where Π is a $m \times m$ permutation matrix.

It is easy to check that whenever $U \in GL_n(d)$, W is a permutation of E , and V is an arbitrary $d \times (m - 1)$ integer matrix, then T is a symmetry of \mathcal{M} . Let us call this group of symmetries Γ , and use its members to act on elements of \mathcal{M} by $\mathbf{k} \mapsto T\mathbf{k}$ or elements of $\mathcal{R}(\lambda)$ by $J \mapsto J \circ T$. We conjecture that for any $\lambda > 0$, $\mathcal{R}(\lambda)$ has finitely many faces (in particular vertices) up to the action of Γ , but we do not have a proof, except in the cases where we have enumerated the vertices (see Sec. 4), and found, by the fact of the algorithm halting, that there were finitely many vertices.

2.5. The rank constraint

Equation (5) described how to obtain a quadratic form $J \in \mathcal{R}(\lambda)$ from an m -periodic packing Ξ of packing radius $\rho(\Xi) \geq \frac{1}{2}\lambda^{1/2}$. However, the reverse operation is not always possible. Clearly, $\text{rank } J = d$ is a necessary condition. In fact, it is also sufficient, since $J \in \mathcal{R}(\lambda)$ for $\lambda > 0$ implies that Q is positive definite, and therefore $\mathbf{a}_1, \dots, \mathbf{a}_d$ can be recovered through, e.g., Cholesky decomposition, and $\mathbf{b}_1, \dots, \mathbf{b}_{m-1}$ by solving $R_{ij} = \mathbf{b}_i \cdot \mathbf{a}_j$.

Let $\mathcal{R}_0(\lambda) = \{J \in \mathcal{R}(\lambda) : \text{rank } J = d\}$. For $m = 2$, we can replace the condition $\text{rank } J = d$ by $\det J = 0$ or $\lambda_{\min}(J) = 0$, where λ_{\min} denotes the smallest eigenvalue. In general, we can write it as the vanishing of the Schur complement $S - RQ^{-1}R^T = 0$.

2.6. The density objective

We wish to find the maximum of $\delta(\Xi)$ among m -periodic sets Ξ of packing radius at least ρ_0 . This is equivalent to finding the minimum of $f(J) = \det Q$ among $J \in \mathcal{R}_0(4\rho_0^2)$, where Q is the top-left block of J . While $f(J)$, like the objective in Voronoi's algorithm, is quasiconcave, the nonlinearity of the rank constraints does not allow for a straightforward characterization of the local minima.

A vivid illustration of a new type of local minima that can arise is the 9-dimensional fluid diamond packing, $D_9^+(\mathbf{t}) = D_9 \cup (D_9 + \mathbf{t})$. The lattice $D_9 = \{\mathbf{n} \in \mathbb{Z}^9 : n_1 + n_2 + \dots + n_9 \in 2\mathbb{Z}\}$ has a packing radius $\rho = 1/\sqrt{2}$ and is an extreme lattice, so that any nearby lattice has a smaller packing radius or a larger determinant. However, the hole centered at $(\frac{1}{2}, \frac{1}{2}, \dots, \frac{1}{2})$ is at a distance $3/2 > 2\rho$ from the closest lattice point, and so when \mathbf{t} is in the neighborhood of this deep hole, $D_9^+(\mathbf{t})$ also has packing radius $\rho = 1/\sqrt{2}$. As a 2-periodic point set, this is clearly a local maximum of the density since a nearby 2-periodic point set would have a lattice of symmetry nearby the D_9 lattice and therefore a smaller packing radius or a larger determinant. Thus we have a 9-dimensional family of locally optimal 2-periodic point sets, which achieves the highest known packing density for spheres in 9 dimensions. (In fact, the set of values of \mathbf{t} such that the packing radius is $1/\sqrt{2}$ connects all the deep holes of D_9 , and the two lattices can flow past each other an unbounded distance). A similar situation in a lower dimension can be constructed using the extreme A_8 lattice and its deep hole.

This vivid example should discourage us from attempting to transport the methods of the Voronoi algorithm, where a critical result was that all local optima lie on vertices and are therefore isolated. However, we will show that, at least in the case $m = 2$, the fluid diamond example illustrates the only possible problem we may encounter. Namely, for $m = 2$, a local optimum of $f(J)$ in $\mathcal{R}_0(\lambda)$ either lies on an edge of $\mathcal{R}(\lambda)$ or is part of a fluid family, where two copies of a constant extreme lattice flow relative to each other.

To start, we define a sufficient condition for local optimality by linearizing

all of the constraints, which we call *algebraic extremeness*, and prove that it is indeed a sufficient condition. Let $J \in \mathcal{R}_0(\lambda)$. The set $\{J' : \text{rank } J' = d\}$ is a $[\frac{1}{2}(d+m)(d+m-1) - \frac{1}{2}m(m-1)]$ -dimensional manifold in the neighborhood of J , and its tangent space is given by

$$T_J = J + (\mathcal{S}[N(J)])^\perp = \{J' : \langle J' - J, \mathbf{u}\mathbf{u}^T \rangle = 0 \text{ for all } \mathbf{u} \in N(J)\},$$

where $N(J)$ is the null space of J , and $\mathcal{S}[N(J)]$ is the space of quadratic forms over $N(J)$. The linear inequality constraints, encoded in the polyhedron $\mathcal{R}(\lambda)$, give rise in the neighborhood of J to the cone

$$C_J = \{J' : J'(\mathbf{k}) \geq \lambda \text{ for all } \mathbf{k} \in \mathcal{M} \text{ such that } J(\mathbf{k}) = \lambda\}.$$

Finally, the gradient of the objective is proportional to

$$G_J = \begin{pmatrix} Q^{-1} & 0 \\ 0 & 0 \end{pmatrix}.$$

Definition 1. A configuration $J \in \mathcal{R}_0(\lambda)$ is called *algebraically extreme* if $\langle J' - J, G_J \rangle > 0$ for all $J' \in C_J \cap T_J$ except $J' = J$.

Theorem 2. Let $J \in \mathcal{R}_0(\lambda)$ be algebraically extreme. Then

1. J is an isolated minimum of $f(J')$ among $J' \in \mathcal{R}_0(\lambda)$.
2. J lies on a $\frac{1}{2}m(m+1)$ -dimensional face of $\mathcal{R}(\lambda)$.

Proof. The first claim follows as the usual sufficient optimality criterion for a smooth optimization problem with smooth equality and inequality constraints [14].

To prove the second claim, note that if J lies on a r -dimensional face of $\mathcal{R}(\lambda)$ (considering the polyhedron itself as a full-dimensional face) and $r > \frac{1}{2}m(m+1)$, then C_J contains an affine space passing through J of dimension r . Since T_J is an affine space of codimension $\frac{1}{2}m(m+1)$ passing through J , then $C_J \cap T_J$ must include a positive-dimensional affine subspace, and it is not possible for $\langle J' - J, G_J \rangle$ to be positive everywhere on this subspace, even with J excepted. Therefore, J is not algebraically extreme. \square

Definition 2. A configuration $J \in \mathcal{R}_0(\lambda)$ is called a *fluid packing* if it sits on a continuous, nonconstant curve $J': [0, 1] \rightarrow \mathcal{R}_0(\lambda)$, such that $J'(0) = J$, the upper-left block $Q'(t)$ is constant, and $J'(t)$ is a local minimum of f over $\mathcal{R}_0(\lambda)$ for all $0 \leq t \leq 1$.

Theorem 3. Let $m = 2$, and let $J \in \mathcal{R}_0(\lambda)$. If J is a local minimum of $f(J')$ among $J' \in \mathcal{R}_0(\lambda)$ then one of the following is true:

1. J is algebraically extreme.
2. J is a fluid packing.

Proof. Without loss of generality, let $\lambda = 4$. Let $\{\mathbf{k}_1, \dots, \mathbf{k}_s\} = \{\mathbf{k} : J(\mathbf{k}) = 4\} = J^{-1}(4)$. The quadratic form J is a local optimum of the problem

$$\begin{aligned} & \text{Minimize } f(J'), \\ & \text{subj. to } g_i(J') \triangleq 4 - \langle \mathbf{k}_i \mathbf{k}_i^T, J' \rangle \leq 0 \text{ for } i = 1, \dots, s, \\ & h(J') \triangleq \lambda_{\min}(J') = 0. \end{aligned} \tag{10}$$

As a consequence, it satisfies the Karush-Kuhn-Tucker condition. Namely, there exist $u_{\mathbf{k}} \geq 0$ and v such that $\nabla f + \sum_{i=1}^s u_i \nabla g_i + v \nabla h = 0$. We consider the derivative with respect to $J'_{d+1, d+1}$, which we denote $\partial_{d+1, d+1}$. Since $\partial_{d+1, d+1} f = 0$, $\partial_{d+1, d+1} g_i \leq 0$, and $\partial_{d+1, d+1} h > 0$, we have that $v \geq 0$. The Lagrangian corresponding to these KKT coefficients is $L = f + \sum u_i g_i + v h$. Let C_0 be the marginal cone

$$\begin{aligned} C_0 &= \{ \tilde{J} : \langle \nabla g_i, \tilde{J} \rangle = 0 \text{ for all } i \in I^+, \\ & \quad \langle \nabla g_i, \tilde{J} \rangle \geq 0 \text{ for all } i \in I^0, \\ & \quad \langle \nabla h, \tilde{J} \rangle = 0 \}, \end{aligned} \tag{11}$$

where $I^+ = \{i : u_i > 0\}$ and $I^0 = \{i : u_i = 0\}$. Suppose that J is not algebraically extreme, then the marginal cone is nontrivial. Consider the Hessian of the Lagrangian $H = \text{hess } L = \text{hess } f + v \text{hess } h$, where, e.g., $\langle \tilde{J}, (\text{hess } f) \tilde{J} \rangle = (d^2/dt^2)f(J + t\tilde{J})$. A necessary condition for J to be a local optimum of (10) is that $\langle \tilde{J}, H \tilde{J} \rangle$ is nonnegative for all $\tilde{J} \in C_0$ [14, p. 216]. However, both $\text{hess } f$ and $\text{hess } h$ are negative semidefinite (for f , this is the quasiconcavity

of the determinant function; for h , this is a well-known result of second-order eigenvalue perturbation theory). It follows that C_0 must lie in the null-space of $\text{hess } f$, that is, the Q component of any vector in the marginal cone is zero.

Consider a nonzero element $\tilde{J} \in C_0$, with blocks $\tilde{Q} = 0$, \tilde{R} , and \tilde{S} , and let $J'(t)$ be a one-parameter family such that $Q'(t) = Q$, $R'(t) = R + t\tilde{R}$, and $S'(t) = S + t\tilde{S} + t^2\tilde{R}^T Q^{-1} \tilde{R}$. By the Schur complement condition, we see that $\text{rank } J'(t) = d$ for all t . Also, $g_i(J'(t)) = 4 - \mathbf{k}_i^T J'(t) \mathbf{k}_i = \langle \nabla g_i, \tilde{J} \rangle - t^2 \mathbf{1}^T \tilde{R}^T Q^{-1} \tilde{R} \mathbf{1}$ is nonpositive for $t > 0$ by the positive definiteness of Q^{-1} . Therefore, for some ϵ , $J'(t) \in \mathcal{R}_0(4)$ for all $0 \leq t < \epsilon$. Since $f(J'(t)) = f(J)$ and J is a local minimum of f over $\mathcal{R}_0(4)$, so must $J'(t)$ for all sufficiently small t . Therefore J is a fluid packing. \square

Theorems 2 and 3 suggest a straightforward generalization of Voronoi's algorithm to 2-periodic sets, which we elaborate in the next section.

3. The generalized Voronoi algorithm

3.1. Outline

Our algorithm seeks to enumerate all the locally optimal 2-periodic sets in d dimensions. As we proved in Theorem 3, those are either fluid packings or algebraically extreme packings. The problem of enumerating the fluid packings is rather straightforward for $m = 2$, since the two component lattices must themselves be extreme. Therefore, for each extreme d -dimensional lattice, each hole (circumcenter of Delone cell) that is deep enough to accommodate another translate of the lattice without reducing the packing radius can give rise to a fluid packing, and these different fluid packings may or may not be connected to each other via their flow. This informal description is the extent to which we will discuss this part of the problem in this paper, and we will devote the remainder to the enumeration of the algebraically extreme lattices. In fact, in the dimensions where we have implemented our algorithm and present the results of the full enumeration, there are no fluid packings.

The enumeration of the algebraically extreme 2-periodic sets of packing radius 1 consists of two steps that can be conceptually thought of as occurring one after the other, but in our implementation are actually interleaved. The first step is to enumerate all the vertices and edges of $\mathcal{R}(4)$ up to equivalence under the action of Γ . The second step is to take each edge, represented in the form $\{J + tJ' : 0 \leq t \leq 1\}$ or $\{J + tJ' : t \geq 0\}$, solve for all t such $J + tJ' \in \mathcal{R}_0(4)$, and check whether $J + tJ'$ is algebraically extreme. We elaborate on these steps below.

3.2. The shortest vector problem and related problems

Throughout the algorithm, we need to solve a problem analogous to the problem known as the shortest vector problem (SVP) in the context of lattices [15]. In our context, given a quadratic form $J : \mathbb{R}^{d+m-1} \rightarrow \mathbb{R}$ with positive definite upper-left $d \times d$ block Q , we wish to find its minimum over nonzero vectors in $\mathcal{M} = \mathbb{Z}^d \times (E - E)$. We also, in some cases, want to enumerate the vectors attaining this minimum, or more generally enumerate all vectors that attain a value below some threshold.

For $\mathbf{k} = (\mathbf{n}, \mathbf{l}) \in \mathcal{M}$ with fixed \mathbf{l} , $J(\mathbf{k})$ is an inhomogeneous quadratic form of \mathbf{n} (see Eq. (7)). Finding the minimum of an inhomogeneous quadratic form over the integer vectors is a problem known as the closest vector problem (CVP) for lattices and is closely related to the SVP [15]. Since there are only finitely many possible values of \mathbf{l} , we have thus reduced the SVP problem for m -periodic forms to a finite number of instances of the CVP problem for the underlying lattice.

As in the case of lattices, it might be expected that reduction of the quadratic form (using elements of Γ) would significantly decrease the average time to compute the SVP. To reduce the form, we first reduce the underlying lattice (the Q block) by applying an operation T of the form (8), where $V = 0$ and $W = 1$. We then perform size reduction of the translation vectors, by applying the appropriate operation T , where $U = 1$ and $W = 1$, so that $Q^{-1}R^T$ has entries in $[-\frac{1}{2}, \frac{1}{2}]$.

3.3. Enumeration of vertices

The algorithm to enumerate the vertices of $\mathcal{R}(4)$ is similar to the one accomplishing the analogous task in Voronoi's algorithm. We start with a known vertex of $\mathcal{R}(4)$, denoted J_1 . We compute the extreme rays of its cone C_{J_1} [16]. For each such ray, $\{J_1 + tJ' : t \geq 0\}$ there are two possibilities: either it lies entirely in $\mathcal{R}(4)$ or there is some $t > 0$ such that $J_1 + tJ'$ is another vertex of $\mathcal{R}(4)$, which we say is *contiguous* to J_1 . The first possibility does not exist in the original algorithm for lattices, but does occur in our case, and we must check for this possibility. We discuss this problem in Section 3.4.

For each contiguous vertex, we check if it is equivalent to J_1 (more on this step in Section 3.5), and if not, we add it to a queue of vertices to be processed and to our partial enumeration of vertices. At each subsequent step of the algorithm, we remove a vertex from the queue, compute its contiguous vertices, check them for equivalence against all vertices in our partial enumeration, and add the ones that are not equivalent to previously enumerated vertices to the queue and to the partial enumeration. The enumeration is complete when the queue is empty. Since vertices of $\mathcal{R}(4)$ are necessarily rational, we can perform these calculations using exact arithmetic.

One way to obtain a starting vertex to initialize the algorithm is as follows: consider A_d (or D_d , or any extreme, nonfluid d -dimensional lattice). It can be represented as 2-periodic set by taking a sublattice of index 2 instead of the primitive lattice. This 2-periodic set is necessarily algebraically extreme [13], and so it lies on an edge of $\mathcal{R}(4)$, which must terminate at a vertex in at least one direction.

3.4. Detection of unbounded edges

Given a vertex J of $\mathcal{R}(4)$ and an extreme ray of C_J , of the form $\{J + tJ' : t \geq 0\}$, we want to determine if the ray lies entirely in $\mathcal{R}(4)$. This is the case if and only if $J'(\mathbf{k}) \geq 0$ for all $\mathbf{k} \in \mathcal{M}$. So, we have a problem very similar to the SVP above, except that we may not assume that Q' is positive definite. If Q' is not even positive semidefinite, then there is some $\mathbf{k} = (\mathbf{n}, 0)$ such that

$J'(\mathbf{k}) = Q'(\mathbf{n}) < 0$, and the ray is not unbounded. So the only remaining case is when Q' is positive semidefinite and has nontrivial null space, $N(Q')$.

We break this remaining case into two cases. First, consider the case that there exist $\mathbf{l} \in (E - E)$ and $\mathbf{u} \in N(Q')$ with $c = \mathbf{u}^T(R')^T\mathbf{l} > 0$. Let $\mathbf{v}(t) = (-tc\mathbf{u}, \mathbf{l})$, let $[\mathbf{v}](t) \in \mathcal{M}$ be the closest integer vector to $\mathbf{v}(t)$, and let $(\mathbf{e}, 0) = \mathbf{v}(t) - [\mathbf{v}](t)$ be the remainder. Then

$$J'([\mathbf{v}](t)) = t^2 c^2 \mathbf{u}^T Q' \mathbf{u} - tc \mathbf{u}^T Q' \mathbf{e}^T + \mathbf{e} Q' \mathbf{e} - 2tc^2 + \mathbf{l}^T S \mathbf{l}. \quad (12)$$

All terms except $-2tc^2$ are either zero or bounded as $t \rightarrow \infty$ and so $J'([\mathbf{v}](t)) < 0$ for large enough t and the ray is not unbounded.

The final case is that $\mathbf{u}^T(R')^T\mathbf{l} = 0$ for all $\mathbf{l} \in (E - E)$ and $\mathbf{u} \in N(Q')$. In this case, the problem reduces to the first case, where Q' is positive definite, albeit in a smaller dimension: Since Q' is a rational matrix, there a unimodular transformation $U \in GL_d(\mathbb{Z})$ such that $Q' \circ U$ has span $\{\mathbf{e}_{r+1}, \dots, \mathbf{e}_d\}$ as its null space and is positive definite on span $\{\mathbf{e}_1, \dots, \mathbf{e}_r\}$. We can find this transformation by computing the Hermite normal form or the Smith normal form of Q' scaled to an integer matrix. Let $\mathbf{n} = \mathbf{n}' + \mathbf{n}''$ with $\mathbf{n}'' \in N(Q' \circ U)$ and $\mathbf{n}' \in N(Q' \circ U)^\perp$. Then

$$J'(U(\mathbf{n}), \mathbf{l}) = (\mathbf{n}')^T U^T Q' U \mathbf{n} + 2(\mathbf{n}')^T U^T (R')^T \mathbf{l} + 2(\mathbf{n}'')^T U^T (R')^T \mathbf{l} + \mathbf{l}^T S \mathbf{l}. \quad (13)$$

Since, by assumption of this case, $(\mathbf{n}'')^T U^T (R')^T \mathbf{l} = 0$, the value of $J'(U(\mathbf{n}), \mathbf{l})$ depends only on \mathbf{n}' and \mathbf{l} , and we may find its minimum using our SVP method.

3.5. Equivalence checking

Given two quadratic forms J_1 and J_2 , we wish to determine if $J_2 = J_1 \circ T = T^T J_1 T$ for some $T \in \Gamma$. Let us denote this relation as $J_1 \sim J_2$. This problem may apply to vertices of $\mathcal{R}(4)$, as part of the algorithm for enumerating vertices, but we may also apply it to any pair of quadratic forms in $\mathcal{R}(4)$ that are not necessarily vertices. Let us first prove some useful results.

Definition 3. A set $M \in \mathcal{M}$ is *perfect* if $J(\mathbf{k}) = J'(\mathbf{k})$ for all $\mathbf{k} \in M$ implies $J = J'$.

A set M is perfect if and only if the set $\{\mathbf{k}\mathbf{k}^T : \mathbf{k} \in M\}$ spans the space of symmetric $(d+m-1) \times (d+m-1)$ matrices. Denote by $J^{-1}(A) \subset \mathcal{M}$ the set of vectors in \mathcal{M} attaining values in the set A . If $A = \{4\}$ and J is a vertex of $\mathcal{R}(4)$, then $J^{-1}(A)$ is perfect. A direct consequence of the definition of a perfect set is the following lemma:

Lemma 2. *Let A be a set of real values, and let $M_1 = J_1^{-1}(A)$ and $M_2 = J_2^{-1}(A)$ be the set of vectors in \mathcal{M} that achieve these values. If M_1 and M_2 are perfect, then the following are equivalent:*

1. $J_2 = J_1 \circ T$ for some $T \in \Gamma$.
2. $T(M_2) = M_1$, and $J_2|_{M_2} = (J_1 \circ T)|_{M_2}$ for some $T \in \Gamma$.

In particular a T that satisfies one condition also satisfies the other.

Proof. First, suppose $J_2 = J_1 \circ T$, and let $\mathbf{k} \in M_2$. Since $J_2(\mathbf{k}) = J_1(T\mathbf{k}) \in A$, we have that $T\mathbf{k} \in M_1$. Similarly, if $\mathbf{k} \in M_1$, then $T^{-1}\mathbf{k} \in M_2$. So $T(M_2) = M_1$, and clearly $J_2|_{M_2} = (J_1 \circ T)|_{M_2}$ follows *a fortiori* from the unrestricted equality.

The other direction follows immediately from the definition of a perfect set. \square

Therefore, a simple algorithm to check for equivalence is as follows: first, construct a set A such that $M_1 = J_1^{-1}(A)$ is perfect. When J_1 is a vertex of $\mathcal{R}(4)$, the set $A = \{4\}$ suffices. Otherwise, we find the smallest $a > 4$ such that $A = [4, a]$ suffices. Next, compute $M_2 = J_2^{-1}(A)$. If M_2 is not perfect, $|M_1| \neq |M_2|$, or J_2 does not take values in A over M_2 with the same frequency as J_1 does over M_1 , then $J_1 \not\sim J_2$. We give labels $1, \dots, s$ to the elements of $M_1 = \{\mathbf{k}_1, \dots, \mathbf{k}_s\}$ and $M_2 = \{\mathbf{k}'_1, \dots, \mathbf{k}'_s\}$, such that $\mathbf{k}_1, \dots, \mathbf{k}_{d+m-1}$ are linearly independent (there must be such a linearly independent subset for M_1 to be perfect). We now try to construct an injective map $\sigma : \{1, \dots, d+m-1\} \rightarrow \{1, \dots, s\}$ such that

$$(\mathbf{k}'_{\sigma(i)})^T J_2 \mathbf{k}'_{\sigma(j)} = \mathbf{k}_i^T T^T J_1 T \mathbf{k}_j \text{ for all } 1 \leq i, j \leq d+m-1. \quad (14)$$

We can do this by a backtracking search, constructing σ on $1, \dots, n < d+m-1$ for increasing n , and backtracking when no possible assignment of $\sigma(n+1)$

satisfies (14) for $1 \leq i, j \leq n+1$. For each such complete map produced by the backtracking search, there is a unique linear map T' such that $T'\mathbf{k}_i = \mathbf{k}'_{\sigma(i)}$ for $1 \leq i \leq d+m-1$. If $T' \in \Gamma$ and $T'(M_1) = M_2$, we are done and $J_1 \sim J_2$. Otherwise, we continue with the backtracking search. If the backtracking search concludes without finding any equivalence, then $J_1 \not\sim J_2$.

3.6. Enumeration of algebraically extreme forms

Given an edge of $\mathcal{R}(4)$ of the form $J + tJ'$, where $0 \leq t \leq 1$ or $t \geq 0$, we wish to identify the points of this edge that lie in $\mathcal{R}_0(4)$. As we are limiting ourselves to the case $m = 2$, we simply need to solve $\det(J + tJ') = 0$ for t , which is a univariate polynomial equation. This equation can be solved for t as a generalized eigenvalue problem $J\mathbf{x} = -tJ'\mathbf{x}$. It is possible that the entire edge lies in $\mathcal{R}_0(4)$, as happens for one edge in our enumeration for $d = 5$. In that case, either Q is constant over the edge, and any locally optimal packing on the edge is necessarily a fluid packing, or Q is not constant, and therefore neither is f , so only points that minimize f over the edge — necessarily endpoints by quasiconcavity — can be locally optimal packings. In any case, we have a finite number of points for which we need to determine if they are algebraically extreme.

Given $J \in \mathcal{R}(4)$, we can certify that it is algebraically extreme by looking at the dual problem. Namely, J is algebraically extreme if and only if the cone $\{\sum_{\mathbf{k} \in J^{-1}(4)} \eta_{\mathbf{k}} \mathbf{k} \mathbf{k}^T + \mathbf{x} \mathbf{x}^T : \eta_{\mathbf{k}} > 0, \mathbf{x} \in N(J)\}$ is full-dimensional and includes G_J . Otherwise, we can certify the opposite by the direct problem of finding J' that gives a counterexample for the definition: $J' \neq J$, $\langle J' - J, G_J \rangle \leq 0$, and $J' \in C_J \cap T_J$. Since t comes from the root of a univariate polynomial, it is not, in general, rational. In our calculation, we use floating point representation for the candidate algebraic extreme sets.

4. Numerical results

We use an implementation of the algorithm described in the previous section to fully enumerate the vertices of the Ryshkov-like polyhedron $\mathcal{R}(4)$ and the

vertices of $\mathcal{R}(4)$	4 (2)	10 (6)	34 (25)
algebraically extreme 2-periodic sets	3 (1)	7 (3)	29 (20)
highest density	$1/(2\sqrt{2})$	$1/8$	$1/(8\sqrt{2})$
multiplicity of highest density	3 (1)	2 (0)	5 (2)

Table 1: Summary of enumeration results. For $d = 3, 4, 5$ we list the number of vertices of the Ryshkov-like polyhedron, the number of algebraically extreme 2-periodic sets, the highest number density achieved for packing radius 1, and the number of algebraically extreme sets that achieve this density. In parentheses, we indicate how many of the corresponding 2-periodic sets are not also lattices.

algebraically extreme m -periodic sets for $m = 2$ and $d = 3, 4, 5$. Our attempted enumeration for $d = 6$ did not terminate after over a month of running. The main bottleneck appears to be the enumeration of extreme rays of C_J for vertices J with large number of minimal vectors $J^{-1}(4)$ (see Sec. 4.4). This is similar to the main bottleneck in the enumeration of perfect lattices in $d = 8$, where only by exploiting the symmetries of these high-kissing-number lattices, was the full enumeration made tractable [17]. We are hopeful that a similar approach could be used for $m = 2$ to make full enumeration in higher dimensions than $d = 5$ tractable, but we do not attempt to implement it in this work.

4.1. $d=3$

The enumeration in $d = 3$ gave 4 inequivalent vertices and 3 inequivalent algebraically extreme 2-periodic sets. All the algebraically extreme 2-periodic sets in 3 dimensions of packing radius 1 have the same density $\delta = 1/(2\sqrt{2}) \approx 0.354$, and they are represented by the following quadratic forms:

$$J_{3,1} = 2 \begin{pmatrix} 2 & 0 & 0 & -1 \\ 0 & 2 & 0 & 1 \\ 0 & 0 & 4 & 2 \\ -1 & 1 & 2 & 2 \end{pmatrix} \quad J_{3,2} = 2 \begin{pmatrix} 2 & -1 & 1 & 0 \\ -1 & 2 & 0 & 1 \\ 1 & 0 & 6 & 3 \\ 0 & 1 & 3 & 2 \end{pmatrix} \quad (15)$$

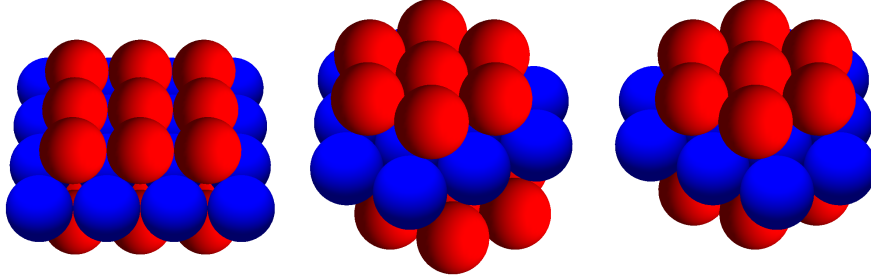


Figure 1: The three algebraically extreme 2-periodic packings in 3 dimensions. We use red and blue spheres to represent the two orbits under translation by lattice vectors. Both the left and middle packings are representations of the fcc lattice as a 2-periodic set, but they are not equivalent when the two orbits are distinguished. The right packing is the hexagonal close-packed 2-periodic arrangement and is the only algebraically extreme 2-periodic packing in 3 dimensions that is not also a lattice.

$$J_{3,3} = \frac{2}{3} \begin{pmatrix} 6 & 3 & 0 & 0 \\ 3 & 6 & 0 & 3 \\ 0 & 0 & 16 & 8 \\ 0 & 3 & 8 & 6 \end{pmatrix} \quad (16)$$

The forms $J_{3,1}$ and $J_{3,2}$ are two inequivalent representations of the fcc lattice as a 2-periodic set. $J_{3,1}$ is a stacking of square layers, whereas $J_{3,2}$ is a stacking of triangular layers (see Figure 1). The forms are not equivalent under the action of Γ because the corresponding two sublattices of the fcc lattices are not equivalent under the symmetries of the fcc lattice. The form $J_{3,3}$ represents the hexagonal-close-packing 2-periodic arrangement, which is not a lattice. Note that a form J is the representation of a lattice as a 2-periodic set if and only if $Q^{-1}R^T \in (\frac{1}{2}\mathbb{Z})^d$.

All the algebraically extreme 2-periodic sets have the same kissing number, 12, but as quadratic forms they have different number of minimal vectors: $|J_{3,1}^{-1}(4)| = 20$, $|J_{3,2}^{-1}(4)| = |J_{3,3}^{-1}(4)| = 18$. This difference occurs because contacts between spheres in the same orbit contribute the same minimal vector as the analogous contact in a different orbit. Denote by $|\cdot|_*$ a counting measure

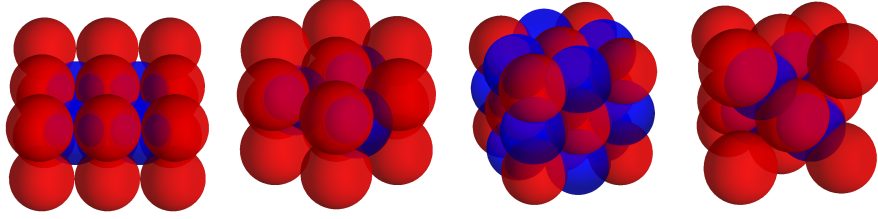


Figure 2: The vertices of the Ryshkov-like polyhedron for $d = 3$ and $m = 2$ can be interpreted as binary packings of nonadditive hard spheres.

that gives weight m to vectors of the form $\mathbf{k} = (\mathbf{n}, 0)$. Then the average kissing number is $\kappa = |J^{-1}(\min J)|_*/m$.

The vertices of the Ryshkov-like polyhedron are also interesting to consider. They are

$$J_{3,1v} = 2 \begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & -1 \\ 0 & 0 & 2 & 1 \\ 1 & -1 & 1 & 2 \end{pmatrix} \quad J_{3,2v} = 2 \begin{pmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{pmatrix} \quad (17)$$

$$J_{3,3v} = 2 \begin{pmatrix} 2 & 1 & -1 & 0 \\ 1 & 2 & 0 & 1 \\ -1 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{pmatrix} \quad J_{3,4v} = 2 \begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 1 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 1 & 0 & 2 \end{pmatrix}. \quad (18)$$

They have full rank, so they do not correspond to 2-periodic sets in 3 dimensions. However, because they are positive definite, they correspond to 4-dimensional sets that are periodic (with two orbits) under a 3-dimensional lattice. When they are projected to the space spanned by the lattice, they can be interpreted as binary packings of non-additive spheres, where the two sphere species have equal self-radius, but smaller radius when interacting with each other. The first is a simple cubic lattice of one species with its body-center holes filled with spheres of the other species. The second is a hexagonal lattice with one of the two inequivalent triangular prism-shaped holes in each unit cell filled. The third

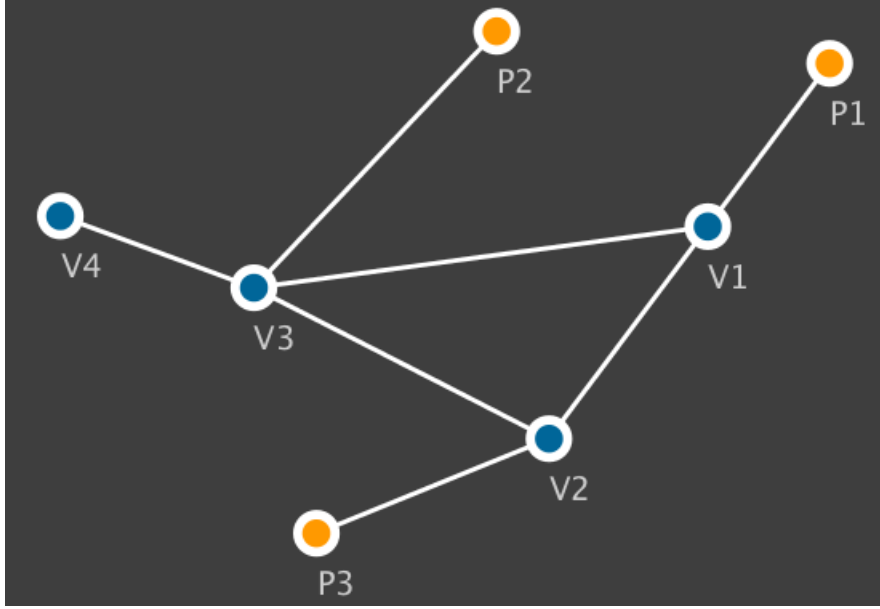


Figure 3: The Voronoi graph of 2-periodic sets in $d = 3$, a generalization of the Voronoi graph for lattices. The blue nodes are the vertices of $\mathcal{R}(4)$, the Ryshkov-like polyhedron; the orange nodes are points of $\mathcal{R}_0(4)$ lying on unbounded edges (rays) of $\mathcal{R}(4)$. Two vertices are connected in the graph if they are contiguous, and edge points are connected to the vertices on which their edge is incident. The labels Vn and Pn corresponds to $J_{3,nv}$ and $J_{3,n}$ respectively. In $d = 3$ all the points of $\mathcal{R}_0(4)$ lying on polyhedron edges are on unbounded edges and they are all algebraically extreme.

and fourth are the fcc lattice with its octahedral or (one of its) tetrahedral holes filled, giving, respectively, a simple cubic lattice with alternating species (the NaCl crystal structure) and the diamond crystal structure (see Figure 2).

Finally, we point out as an example of an unbounded edge, the edge connecting $J_{3,3}$ and $J_{3,2v}$.

4.2. $d=4$

In 4 dimensions, we obtain 7 inequivalent algebraically extreme 2-periodic sets. Six of those lie in the relative interior of edges of the Ryshkov-like polyhedron, and one is a vertex. Two algebraically extreme sets achieve the maximum density, $\delta = 1/8 = 0.125$, and both are representations of the lattice D_4 as a

2-periodic set. They are represented by the forms,

$$J_{4,1} = 2 \begin{pmatrix} 2 & 0 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 & -1 \\ 0 & 0 & 2 & 0 & -1 \\ 0 & 0 & 0 & 2 & -1 \\ 1 & -1 & -1 & -1 & 2 \end{pmatrix} \quad J_{4,2} = 2 \begin{pmatrix} 2 & -1 & -1 & 0 & -1 \\ -1 & 2 & 1 & 0 & 1 \\ -1 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 4 & 2 \\ -1 & 1 & 0 & 2 & 2 \end{pmatrix}. \quad (19)$$

The form $J_{4,1}$ is a vertex of the Ryshkov-like polyhedron. Both have the kissing number of D_4 , $\kappa = 24$, as the average kissing number. The next-highest density achieved is $\delta = 2/\sqrt{144 + 64\sqrt{5}} \approx 0.118$, which is achieved by a single algebraically extreme 2-periodic set:

$$J_{4,3} = 2 \begin{pmatrix} 2 & -1 & -1 & -1 & -1 \\ -1 & 2 & 1 & 1 & 0 \\ -1 & 1 & 2 & 1 & 1 \\ -1 & 1 & 1 & 2 + 2\tau & -\tau \\ -1 & 0 & 1 & -\tau & 2 \end{pmatrix}, \quad (20)$$

where $\tau = (1 + \sqrt{5})/2$ is the golden ratio. Its average kissing number is $\kappa = 22$. Finally, there are four algebraically extreme 2-periodic sets that achieve the same density as the A_4 lattice, $\delta = 1/(4\sqrt{5}) \approx 0.112$. Two of them are in fact representations of the A_4 lattice, but the other two are not also lattices. All four have the same kissing number as the lattice, $\kappa = 20$. Including $J_{4,1}$, there are 10 inequivalent vertices of the Ryshkov-like polyhedron.

4.3. $d=5$

In 5 dimensions, we obtain 29 inequivalent algebraically extreme 2-periodic sets. Five inequivalent 2-periodic sets achieve the maximum density $\delta = 1/(8\sqrt{2}) \approx 0.0884$, three of which are representations of the lattice D_5 as a 2-periodic set, and two are nonlattices that achieve the same density. The ones that represent

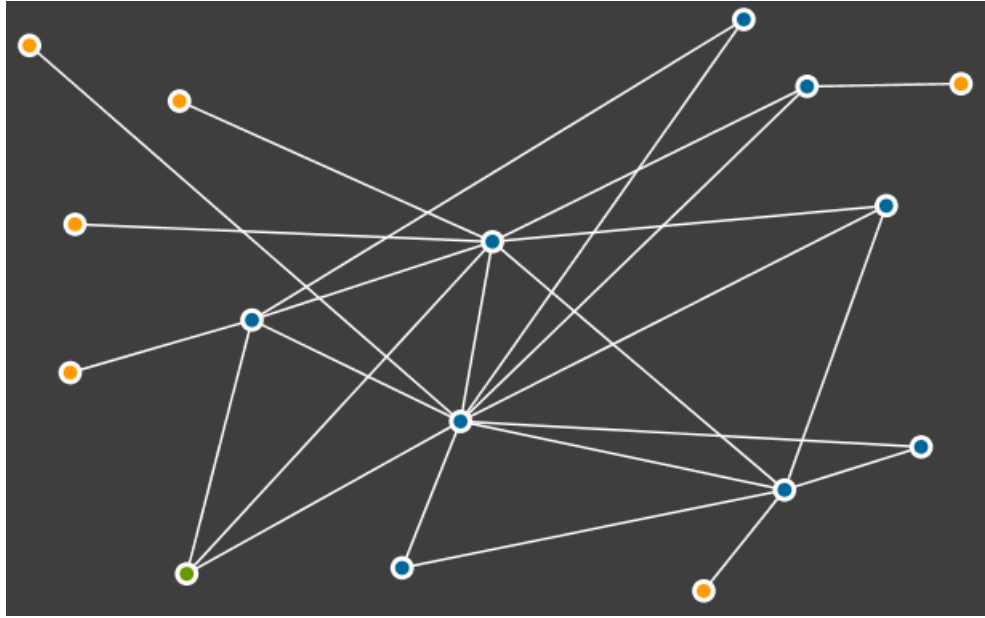


Figure 4: The Voronoi graph in $d = 4$. The blue nodes are polyhedron vertices that are not in $\mathcal{R}_0(4)$. The green and orange nodes are points of $\mathcal{R}_0(4)$ lying on vertices and unbounded edges of the polyhedron, respectively. In $d = 4$, as in $d = 3$, all the points of $\mathcal{R}_0(4)$ in the relative interior of polyhedron edges are on unbounded edges and are all algebraically extreme. We omit the labels for neatness.

the lattice D_5 are given by the forms,

$$J_{5,1} = 2 \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 1 \\ -1 & 2 & 1 & 0 & 0 & 0 \\ -1 & 1 & 2 & 0 & 0 & -1 \\ 0 & 0 & 0 & 2 & 0 & -1 \\ 0 & 0 & 0 & 0 & 2 & -1 \\ 1 & 0 & -1 & -1 & -1 & 2 \end{pmatrix} \quad (21)$$

$$J_{5,2} = 2 \begin{pmatrix} 2 & -1 & -1 & -1 & 0 & -1 \\ -1 & 2 & 1 & 1 & 0 & 1 \\ -1 & 1 & 2 & 0 & 0 & 0 \\ -1 & 1 & 0 & 2 & 0 & 1 \\ 0 & 0 & 0 & 0 & 4 & 2 \\ -1 & 1 & 0 & 1 & 2 & 2 \end{pmatrix} \quad (22)$$

$$J_{5,3} = 2 \begin{pmatrix} 2 & -1 & -1 & -1 & -1 & -1 \\ -1 & 2 & 1 & 1 & 1 & 1 \\ -1 & 1 & 2 & 1 & 1 & 0 \\ -1 & 1 & 1 & 2 & 1 & 1 \\ -1 & 1 & 1 & 1 & 4 & -1 \\ -1 & 1 & 0 & 1 & -1 & 2 \end{pmatrix}, \quad (23)$$

where $J_{5,1}$ is also a vertex of the Ryshkov-like polyhedron (the only vertex that is also in \mathcal{R}_0). The two that are not lattices but achieve the same density are

$$J_{5,4} = \begin{pmatrix} 4 & -2 & -2 & 2 & -2 & -2 \\ -2 & 4 & 0 & -2 & 2 & 0 \\ -2 & 0 & 4 & -2 & 2 & 2 \\ 2 & -2 & -2 & 4 & -2 & -2 \\ -2 & 2 & 2 & -2 & 10 & 5 \\ -2 & 0 & 2 & -2 & 5 & 4 \end{pmatrix} \quad (24)$$

$$J_{5,5} = \frac{2}{5} \begin{pmatrix} 10 & 5 & 5 & -5 & 0 & 0 \\ 5 & 10 & 5 & -5 & 0 & 5 \\ 5 & 5 & 10 & -5 & 0 & 5 \\ -5 & -5 & -5 & 10 & 0 & -5 \\ 0 & 0 & 0 & 0 & 16 & -8 \\ 0 & 5 & 5 & -5 & -8 & 10 \end{pmatrix}. \quad (25)$$

All have the same kissing number $\kappa = 40$.

The next highest density, $\delta = (\sqrt{5 - 2\sqrt{6}})/4 \approx 0.0795$, is achieved by three algebraically extreme 2-periodic sets, all of which are not also lattices:

$$J_{5,6} = \frac{2}{5} \begin{pmatrix} 10 & -5 & -5 & 5 & -5 & -5 \\ -5 & 10 & 5 & -5 & 5 & 0 \\ -5 & 5 & 10 & -5 & 0 & 0 \\ 5 & -5 & -5 & 10 & -5 & -5 \\ -5 & 5 & 0 & -5 & 16 + 4\sqrt{6} & 8 + 2\sqrt{6} \\ -5 & 0 & 0 & -5 & 8 + 2\sqrt{6} & 10 \end{pmatrix} \quad (26)$$

$$J_{5,7} = \frac{2}{5} \begin{pmatrix} 10 & 5 & -5 & -5 & -5 & 10 \\ 5 & 10 & -5 & -5 & 0 & 10 \\ -5 & -5 & 10 & 5 & 0 & -5 \\ -5 & -5 & 5 & 10 & 0 & -5 \\ -5 & 0 & 0 & 0 & 14 + 4\sqrt{6} & 2 + 2\sqrt{6} \\ 10 & 10 & -5 & -5 & 2 + 2\sqrt{6} & 20 \end{pmatrix} \quad (27)$$

$$J_{5,8} = \frac{1}{2} \begin{pmatrix} 8 & 4 & 4 & 0 & -4 & 0 \\ 4 & 8 & 4 & 0 & -4 & 4 \\ 4 & 4 & 8 & 0 & -4 & 4 \\ 0 & 0 & 0 & 8 & 0 & -4 \\ -4 & -4 & -4 & 0 & 8 + 2\sqrt{6} & -4 - \sqrt{6} \\ 0 & 4 & 4 & -4 & -4 - \sqrt{6} & 8 \end{pmatrix}. \quad (28)$$

The first two of these have a kissing number of $\kappa = 35$, and the third has $\kappa = 34$.

The third largest density is that achieved by one of the three extreme lattices

in 5 dimensions, $\delta = 1/(9\sqrt{2}) \approx 0.0786$, and is achieved by five 2-periodic sets, three of which are representations of the lattice, and all have the same kissing number as the lattice. The third extreme lattice, A_5 , has the lowest density of all extreme lattices, $\delta = 1/(8\sqrt{3}) \approx 0.722$, and this density is achieved by seven 2-periodic sets, three of which represent the lattice, and all having the same kissing number as the lattice. This is also the lowest density achieved by any algebraically extreme 2-periodic set, although there is a form of $\mathcal{R}_0(4)$ on an edge of $\mathcal{R}(4)$ that has lower density, but fails to be algebraically extreme.

Including $J_{5,1}$, the Ryshkov-like polyhedron has 34 vertices. Two of the vertices are not positive semidefinite, and this is the lowest dimension where such vertices occur. When interpreted as nonadditive binary sphere packings, these packings would have a nonself-radius larger than the self-radius. In this sense they are similar to the fluid packings (the distance between orbits is larger than the distance within each orbit), but the underlying lattices are not extreme. Another interesting phenomenon that first occurs in 5 dimensions is an edge of $\mathcal{R}(4)$ that is completely contained in $\mathcal{R}_0(4)$. Such an edge is the one connecting $J_{5,1}$ to $J_{5,1} \circ T$, where

$$T = \begin{pmatrix} 1 & 0 & -1 & 0 & -1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (29)$$

as well as all the equivalent edges. Along the edge $J_{5,1} + t(J_{5,1} \circ T - J_{5,1})$, the objective determinant is $f(t) = 512(1 + t - t^2)$, so any internal point cannot be a locally optimal 2-periodic set.

4.4. $d=6$

In $d = 6$ we were only able to perform partial enumeration starting from a vertex incident on the edge on which a representation of A_6 lies. The partial

#	δ	δ	L/N	κ
1	0.0884	$1/(8\sqrt{2})$	L	40
2	0.0884	$1/(8\sqrt{2})$	L	40
3	0.0884	$1/(8\sqrt{2})$	L	40
4	0.0884	$1/(8\sqrt{2})$	N	40
5	0.0884	$1/(8\sqrt{2})$	N	40
6	0.0795	$\sqrt{5-2\sqrt{6}}/4$	N	35
7	0.0795	$\sqrt{5-2\sqrt{6}}/4$	N	35
8	0.0795	$\sqrt{5-2\sqrt{6}}/4$	N	34
9	0.0786	$1/(9\sqrt{2})$	L	30
10	0.0786	$1/(9\sqrt{2})$	L	30
11	0.0786	$1/(9\sqrt{2})$	L	30
12	0.0786	$1/(9\sqrt{2})$	N	30
13	0.0786	$1/(9\sqrt{2})$	N	30
14	0.0771	$\sqrt{419+1011\sqrt{33}}/1024$	N	30
15	0.0765	$-\sqrt{2}+(2\sqrt{5})/3$	N	29
16	0.0765	$-\sqrt{2}+(2\sqrt{5})/3$	N	29
17	0.0758	$3/(2\sqrt{126+4\sqrt{19}\cos\alpha_1-266\cos 2\alpha_1})$	N	30
18	0.0750	$3/40$	N	30
19	0.0748	$1/(36\sqrt{-58+26\sqrt{5}})$	N	26
20	0.0748	$(3\sqrt{3})/((\sqrt{3-4\cos\alpha_2-8\cos 2\alpha_2})(4(5+4\cos\alpha_2)))$	N	28
21	0.0738	$59049/(4\sqrt{x_3})$	N	25
22	0.0737	$5/(48\sqrt{2})$	N	30
23	0.0722	$1/(8\sqrt{3})$	L	30
24	0.0722	$1/(8\sqrt{3})$	L	30
25	0.0722	$1/(8\sqrt{3})$	L	30
26	0.0722	$1/(8\sqrt{3})$	N	30
27	0.0722	$1/(8\sqrt{3})$	N	30
28	0.0722	$1/(8\sqrt{3})$	N	30
29	0.0722	$1/(8\sqrt{3})$	N	30

Table 2: Some invariants of the 29 algebraically extreme 2-periodic sets in five dimensions, including density and kissing number. The L/N column indicates whether this is the representation of a lattice as a 2-periodic set (L) or a truly nonlattice arrangement (N). Here $\alpha_1 = \frac{1}{3}(\tan^{-1}(3\sqrt{762}) - \pi)$, $\alpha_2 = \frac{1}{3}(\tan^{-1}(9\sqrt{47}/17) - \pi)$, $\alpha_3 = \frac{1}{3}(\tan^{-1}(486\sqrt{1077}/5867) - \pi)$, and $x_3 = 8189832078 + 22432320\sqrt{661}\cos\alpha_3 - 35353733064\cos 2\alpha_3 - 3050582422\cos 4\alpha_3 + 6990736\sqrt{661}\cos 5\alpha_3$.

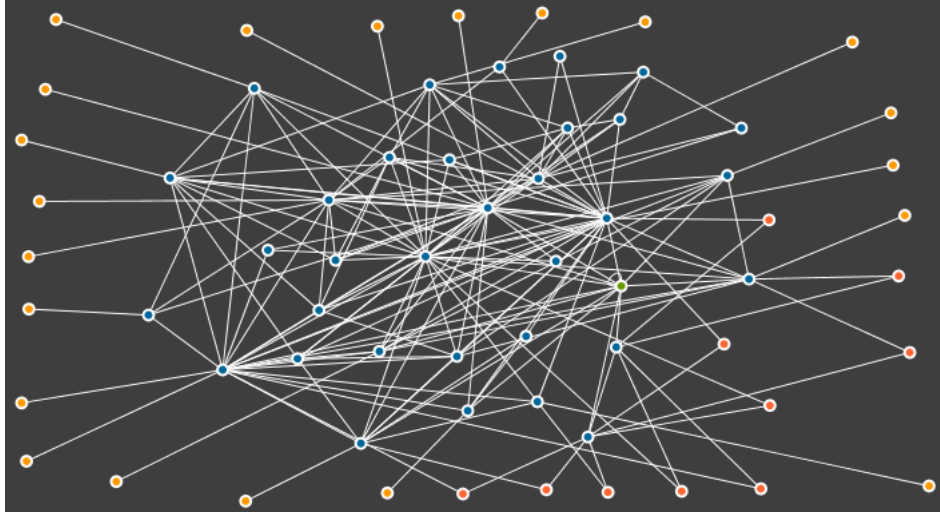


Figure 5: The Voronoi graph in $d = 5$. The notation is the same as in Figs. 3 and 4. This is the lowest dimension where a point of $\mathcal{R}_0(4)$ lying in the relative interior of an edge connecting two vertices appears (red nodes). This is also the lowest dimension where an entire edge of the polyhedron is in $\mathcal{R}_0(4)$, but since only endpoints of such edges can be locally optimal, we do not include such edge points in the graph. We omit the node labels for neatness.

enumeration discovered 730 vertices of $\mathcal{R}(4)$ and 692 points of $\mathcal{R}_0(4)$ on edges of $\mathcal{R}(4)$ (including 8 vertices). There are also 4 edges connecting 3 vertices lying completely in $\mathcal{R}_0(4)$. The obstacles that stalled the full enumeration are three vertices with particularly complex cones. One is a representation of E_6 as a 2-periodic set (with $|J^{-1}(4)| = 124$) and two vertices with $|J^{-1}(4)| = 112$ and $|J^{-1}(4)| = 126$ minimal vectors:

$$J_{6,E_6} = 2 \begin{pmatrix} 6 & -2 & 0 & 0 & 0 & 0 & 3 \\ -2 & 2 & -1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 2 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 2 & 0 \\ 3 & -1 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}, \quad (30)$$

$$J_{6,112} = 2 \begin{pmatrix} 2 & -1 & 1 & -1 & -1 & -1 & 0 \\ -1 & 2 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 2 & -1 & -1 & -1 & 1 \\ -1 & 0 & -1 & 2 & 1 & 1 & -1 \\ -1 & 0 & -1 & 1 & 2 & 1 & 0 \\ -1 & 0 & -1 & 1 & 1 & 2 & 0 \\ 0 & 1 & 1 & -1 & 0 & 0 & 2 \end{pmatrix}, \quad (31)$$

$$J_{6,126} = 2 \begin{pmatrix} 2 & -1 & -1 & -1 & -1 & 1 & -1 \\ -1 & 2 & 1 & 1 & 1 & -1 & 0 \\ -1 & 1 & 2 & 0 & 0 & -1 & 1 \\ -1 & 1 & 0 & 2 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1 & 2 & -1 & 0 \\ 1 & -1 & -1 & 0 & -1 & 2 & -1 \\ -1 & 0 & 1 & 0 & 0 & -1 & 2 \end{pmatrix}. \quad (32)$$

The number of faces of the cone is half the number of minimal vectors. For comparison, the E_7 lattice (as a 1-periodic set) has 126 minimal vectors, and the enumeration of the extreme rays of its cone is already barely tractable by

brute force. Since these forms are highly symmetric (have large automorphism groups), the number of symmetry orbits of the extreme rays is much smaller than the total number of extreme rays. By using a method that exploits the symmetry of these forms, the calculation would hopefully become tractable. This strategy was successful, for example, in making the enumeration of perfect lattice in $d = 8$ tractable [17].

5. Conclusion

Using our generalization of the Voronoi algorithm to 2-periodic sets, we were able to produce a complete enumeration of the locally optimal 2-periodic sphere packings in dimensions $d = 3, 4$, and 5 . In particular, we show that it is impossible to obtain a higher density using 2-periodic arrangements in these dimensions than is possible with lattices. However, in $d = 3$ and $d = 5$ (but not in $d = 4$), there are nonlattice 2-periodic arrangement that match the optimal lattice packing density.

Our work leaves a number of important open questions, whose solution will enable application of this method to higher values of m and d :

1. We were not able to prove *a priori* that the Ryshkov-like polyhedron must have a finite number of faces (in particular vertices) up to the action of Γ . For $m = 2$ and $d = 3, 4, 5$, this follows directly from the fact that our enumeration halts. However, it would be good to know that the enumeration is always guaranteed to halt for any m and d .
2. Theorem 3 is proven only for $m = 2$, but we conjecture that it holds also for $m > 2$. If this conjecture holds, our algorithm can be immediately extended to $m > 2$. However, it would now involve looking for points of $\mathcal{R}_0(4)$ that lie on $\frac{1}{2}m(m+1)$ -dimensional faces of $\mathcal{R}(4)$. This would significantly increase the complexity of two steps the algorithm. First, instead of enumerating extreme rays of C_J for vertices J , we need to enumerate the $\frac{1}{2}m(m+1)$ -dimensional faces of C_J . Second, instead of

solving for $S - RQ^{-1}R^T = 0$ over a line, we need to solve over a $\frac{1}{2}m(m+1)$ -dimensional space.

3. To make the enumeration for $m = 2$ and $d > 5$ tractable, it would be helpful to make use of the symmetries of highly symmetric vertices. For any vertex J , we need only enumerate the orbits of the extreme rays of C_J under the automorphism group of J , $\text{Aut}(J) \subset \Gamma$. Such methods were used to make the enumeration of perfect lattices tractable in $d = 8$ [17].
4. In dimensions where a full enumeration might not be tractable, heuristic optimization methods could be useful for discovering new packing arrangements as well as providing empirical backing to conjectures about certain arrangements being optimal. Again, in the case of lattices ($m = 1$), such methods have been remarkably successful, reproducing the densest known lattices in up to $d = 20$ dimensions. Stochastic enumeration, traversing the 1-skeleton of the Ryshkov polyhedron by picking a random contiguous vertex at each step [11, 18], can be applied to the Ryshkov-like polyhedron treated here. Sequential linear programming methods [19, 20] and simulated annealing methods [21] can also be used to sample periodic arrangements. Our results and those of Schürmann [12, 13] can be used to certify locally optimal packings found.

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